

**EXOTIC MOLECULES IN SPACE : A COORDINATED ASTRONOMICAL
LABORATORY, AND THEORETICAL STUDY**

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Final Report
for the Period 1 May 1997 through 30 April 2000

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Exotic Molecules in Space: A Coordinated Astronomical, Laboratory and Theoretical Study

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Final Report

Great strides have been made during the past three years in our laboratory investigation of molecules of astrophysical interest. Between 20 and 30 new molecules have been discovered each year of the grant with our ultrasensitive Fourier-transform microwave (FTM) spectrometer, bringing the total found during the last three years to 83. (See Figure.) Six of these have already been discovered by us and colleagues in at least one astronomical source in the Galaxy, and a seventh, the molecular ion HC_3NH^+ , has been detected by a Japanese group at Nobeyama Observatory. It is likely that most or many of the remaining 76 will be found with the powerful radio and far infrared telescopes now under construction or planned. The 32 papers published or submitted during the grant period are listed below.

The discovery of five silicon-carbon chains and one ring, rhomboidal SiC_3 , is particularly noteworthy. These all were found during the last few weeks of 1998. As soon as we had good frequencies in hand we attempted to find SiC_3 , the most interesting of the set, and we quickly detected seven lines at precisely the right frequencies in the molecular shell of the well-known evolved carbon star IRC+10216, one of the best astronomical sources of complex molecules. The identification is quite conclusive; SiC_3 is the sixth and largest ring molecule which has been found in space. A paper describing this discovery has appeared in *Astrophysical Journal Letters* (No. 24 in the references here).

Several comments with respect to all the new molecules should be made:

1. There are probably no mistakes in any of the identifications, since these have been confirmed by the standard, powerful assays and tests used to check spectroscopic identifications: isotopic substitution, quantum calculations of the expected molecular structures, detection of hyperfine structure, Zeeman effect, etc. No one--physicist, chemist, or astronomer--to our knowledge has questioned any of the identifications, which generally are about as secure as identifications can be which are largely based on refined, ultra precise, spectroscopic measurements.

2. The radio laboratory astrophysics of the entire set is complete for the time being, in the sense that essentially all the astronomically interesting radio transitions (including hfs when present) are either directly measured or can now be calculated from the derived spectroscopic constants to better than 1 part per million (or 0.3 km s^{-1} in radial velocity, and often much better than that). Because we now know how to make these molecules in specific quantities in our supersonic molecular beam, the stage is set for further studies in the infrared and visible bands. These further studies, some of which are underway in this laboratory, may be of great value to astrophysics; the molecules we have found, for example, may be carriers of the famous optical diffuse interstellar bands, which have been called the outstanding unsolved problem in astrophysical spectroscopy .

3. Sensitive as they are, our laboratory techniques are far from fundamental limits on sensitivity. By cooling the optics and receiver of our FTM spectrometer to the temperature of liquid nitrogen, 77 K, we achieved a year ago a fourfold increase in sensitivity, important to several of our recent discoveries. By further cooling the crucial components of the spectrometer to the temperature of liquid helium, 4 K, as Saykally for example has done in the infrared, we stand to gain an additional order of magnitude in sensitivity.

4. One of the principal motivations of our research is to close the fairly small mass and size gap, now only a factor of a few, between the smallest postulated interstellar grains and the largest identified interstellar molecules. A remarkable effect which we have observed in some of our laboratory discharge sources may help us to significantly narrow this gap. The laboratory decrement in density between one molecule and the next in a homologous series, say between HC_{15}N and HC_{17}N , is much smaller than that between smaller members of the series, say between HC_5N and HC_7N . In fact, the decrement is almost zero for the two large carbon chains just cited. The reason for this is thought to be the enhanced stability of large clusters to dissociative recombination and other destructive processes, and, if so, a similar effect may occur in space. Large molecules may be easier to find both in the laboratory and in space than once thought.

It was clear from the outset that without a determined effort the flood of new molecular data would overwhelm our ability to analyze and to publish. We have accordingly made a strenuous effort to publish our findings rapidly and completely, and we are happy to report that most of our new molecules have already appeared in the leading journals of astronomy, spectroscopy, and physical chemistry, or are in press and about to appear.

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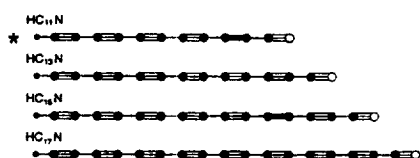
FIGURE CAPTION

The 83 new carbon chains and rings detected with the FTM molecular beam spectrometer during the past three years. The seven identified in space are indicated by an asterisk. The largest carbon chains here have a molecular weight more than twice as large as glycine, the simplest amino acid.

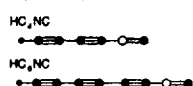
Laboratory Carbon Chains and Rings

Polyynes

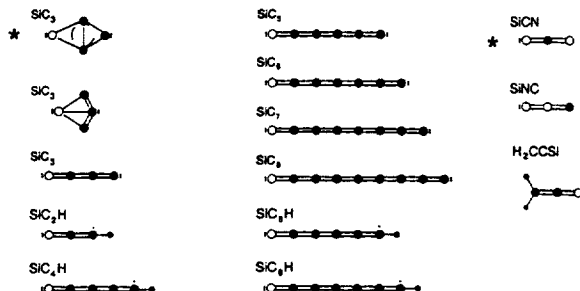
Cyanopolyynes



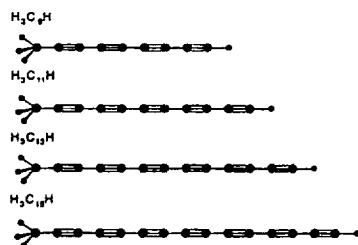
Isocyanopolyynes



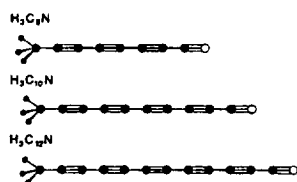
Silicon carbon chains and rings



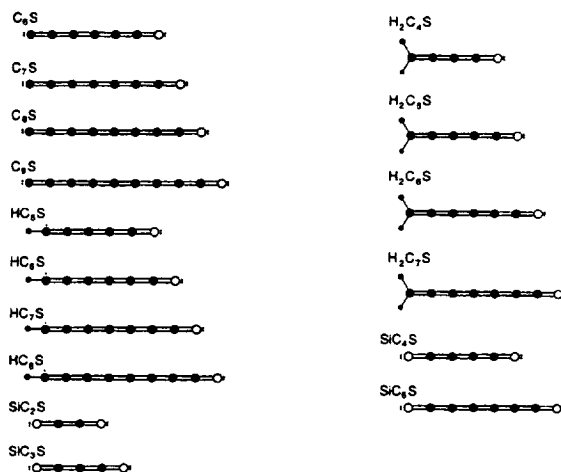
Methylpolyynes



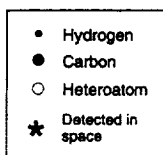
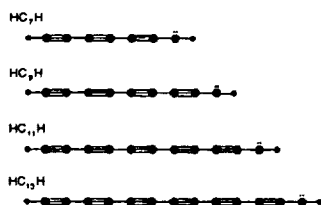
Methylcyanopolyynes



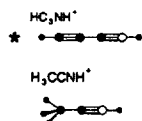
Sulfur carbon chains



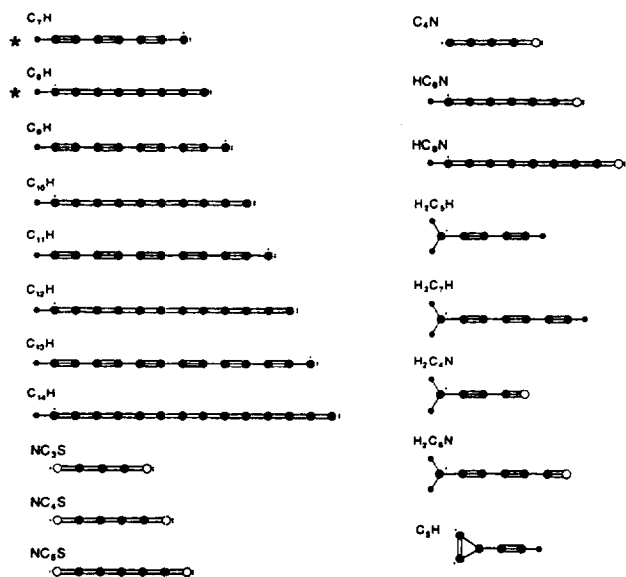
Symmetric carbon chain radicals



Protonated Ions

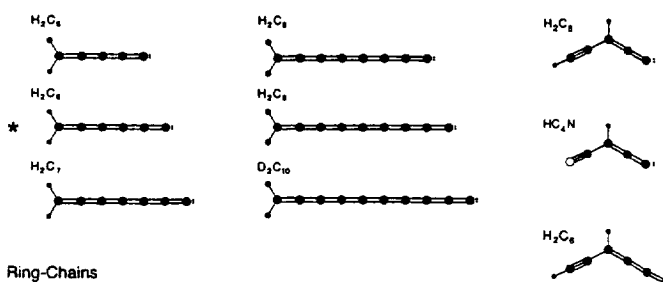


Carbon Chain Radicals



Carbenes

Cumulenes



Ring-Chains

